

VirtualToxLab Results – Praktikum HS 2016/2017

Group 1 (9.11. - 18.11)

Compound	Toxic Potential
CCN.pdb	0.429 ^A
YZ_LC.pdb	0.526 ^D
TCPP.pdb	0.493 ^B
SM_FS.pdb	0.408
TW_RC.pdb	0.494 ^C
SSSS.pdb	0.358
MMVW.pdb	0.493
sk_yg.pdb	0.454
SWAP.pdb	0.463 ^E
LG_SA.pdb	0.478 ^F

ToxPot < 0.50 → **Low**
0.50 < ToxPot < 0.65 → **Medium**
0.65 < ToxPot → **High**

A Original: 0.629 → downscaled due to unsatisfied salt bridges in 2D6 (4), PPARg (2), AR (4), GR (6), hERG (4)
B Original: 0.643 → downscaled due to unsatisfied salt bridges in 3A4 (3), GR (4), hERG (4), MR (4),
C Original: 0.544 → downscaled due to unsatisfied salt bridges in PPARg (4)
D Original: 0.676 → downscaled due to unsatisfied salt bridges in GR (4), hERG (4)
E Original: 0.563 → downscaled due to unsatisfied salt bridges in hERG (5), TRa (5)
F Original: 0.578 → downscaled due to unsatisfied salt bridges in GR (5), hERG (5)